

Package ‘DiffCorr’

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Type Package

Title Analyzing and Visualizing Differential Correlation Networks in Biological Data

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Description A method for identifying pattern changes between 2 experimental conditions in correlation networks (e.g., gene co-expression networks), which builds on a commonly used association measure, such as Pearson's correlation coefficient. This package includes functions to calculate correlation matrices for high-dimensional dataset and to test differential correlation, which means the changes in the correlation relationship among variables (e.g., genes and metabolites) between 2 experimental conditions.

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Depends R (>= 3.5.0), fdrtool, igraph, multtest, pcaMethods

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AraMetLeaves

A metabolite data set from Arabidopsis leaves by GC-TOF/MS

Description

A metabolite data set. The Arabidopsis metabolome of the aerial regions of individual WT plants and the mto1 and tt4 mutants were analyzed by GC-TOF/MS.

Details

50 samples (WT, n = 17; mto1, n = 13; and tt4, n = 20, biological replicates).

A matrix containing 59 metabolites (rows) and 50 observations (columns).

MetaboLights accession no.: MTBLS40

For comparisons with data from roots (Fukushima et al. 2011) we selected 59 commonly-detected metabolites in both datasets using MetMask <http://metmask.sourceforge.net>.

Author(s)

Atsushi Fukushima

References

Miyako Kusano, Atsushi Fukushima et al. BMC Syst Biol 2007 1:53

AraMetRoots

A metabolite data set from Arabidopsis roots by GC-TOF/MS

Description

A metabolite data set. The Arabidopsis metabolome of the roots of individual WT plants and the mto1 and tt4 mutants were analyzed by GC-TOF/MS.

Details

53 root samples (WT, n = 17; mto1 n = 16; and tt4, n = 20, biological replicates).

A matrix containing 59 metabolites (rows) and 53 observations (columns).

MetaboLights accession no.: MTBLS45

For comparisons with data from aerial parts (Kusano, Fukushima et al. 2007) we selected 59 commonly-detected metabolites in both datasets using MetMask <http://metmask.sourceforge.net>.

Author(s)

Atsushi Fukushima

References

Atsushi Fukushima et al. BMC Syst Biol 2011 5:1.

cluster.molecule

Hierarchical clustering of molecules

Description

Cluster molecules

Usage

```
cluster.molecule(  
  data,  
  method = "pearson",  
  linkage = "average",  
  absolute = FALSE  
)
```

Arguments

data	matrix or data frame
method	c("pearson", "spearman", "kendall", "euclidean", "maximum", "manhattan", "canberra", "binary", or "minkowski")
linkage	c("average", "ward", "single", "complete", "mcquitty", "median", "centroid")
absolute	if TRUE, then 1- COR else 1-COR, default is FALSE

Value

an object of class 'hclust'

Author(s)

Atsushi Fukushima

Examples

```
cluster.molecule(as.matrix(t(iris[,1:4])), "pearson", "average")
```

comp.2.cc.fdr

Export differential correlations between two conditions

Description

Export differential correlations of comparison of two correlation matrices

Usage

```
comp.2.cc.fdr(
  output.file = "res.txt",
  data1,
  data2,
  method = "pearson",
  p.adjust.methods = "local",
  threshold = 0.05,
  save = FALSE
)
```

Arguments

output.file	can specify file name of the results exported
data1	data matrix under condition 1
data2	data matrix under condition 2
method	c("pearson", "spearman", "kendall")
p.adjust.methods	c("local", "holm", "hochberg", "hommel", "bonferroni", "BH", "BY", "fdr", "none")

threshold a threshold of significance levels of differential correlation
save exports the results as a text if TRUE (default: FALSE)

Value

data.frame

Author(s)

Atsushi Fukushima

References

Fukushima, A. Gene (2013) 518, 209-214

Examples

```
## Not run:  
data(AraMetRoots)  
AraMetRoots[AraMetRoots==0] <- NA  
AraMetRootsImp <- completeObs(pca(log2(AraMetRoots), nPcs=3, method="ppca"))  
comp.2.cc.fdr(output.file="res.txt", AraMetRootsImp[,1:17], method="spearman",  
              AraMetRootsImp[,18:37], threshold=0.05)  
  
## End(Not run)
```

compcorr	<i>Compare two correlation coefficients</i>
----------	---------------------------------------------

Description

Compare two correlation coefficients using Fisher's Z-transformation

Usage

```
compcorr(n1, r1, n2, r2)
```

Arguments

n1 sample size under condition 1
r1 correlation coefficient under condition 1
n2 sample size under condition 2
r2 correlation coefficient under condition 1

Value

list of result (diff and p-value)

Author(s)

Atsushi Fukushima

References

http://www.fon.hum.uva.nl/Service/Statistics/Two_Correlations.html <http://support.sas.com/ctx/samples/index.jsp?sid=494>
<http://support.sas.com/ctx/samples/index.jsp?sid=494>

Examples

```
compcorr(10, 0.1, 10, 0.9)
```

cor.dist

Additional distance functions correlation distance (1-r)

Description

Additional distance functions Correlation distance (1-r)

Usage

```
cor.dist(data, methods = "pearson", absolute = FALSE)
```

Arguments

data	a data matrix ([data.frame object] row: metabolites, col: samples or replicates)
methods	a character string indicating which correlation coefficient is to be calculated. One of "pearson" (default), "spearman", or "kendall" can be abbreviated.
absolute	TRUE means that absolute value of the correlation coefficient is used (Default: FALSE).

Details

These functions were originally from 'hybridHclust' package. We modified the functions slightly. See also the reference manual in detail.

Value

the resulting correlation matrix

Author(s)

Atsushi Fukushima

Examples

```
cor.dist(as.matrix(t(iris[,1:4])))
```

`cor2.test`*Correlation Test*

Description

Correlation Test

Usage

```
cor2.test(n, r, method = c("pearson", "kendall", "spearman"))
```

Arguments

n	the number of samples
r	the correlation coefficient
method	"pearson" and "spearman" can be used.

Value

p-value

Author(s)

Atsushi Fukushima

References<http://aoki2.si.gunma-u.ac.jp/R/cor2.html>**Examples**

```
cor2.test(30, 0.6)
```

`generate_g`*Generating graph from data matrix*

Description

Generating graph from data matrix

Usage

```
generate_g(  
  data,  
  method = "pearson",  
  cor.thr = 0.6,  
  neg.flag = 1,  
  node.col = "red",  
  node.size = 7,  
  edge.col = "blue",  
  edge.width = 3  
)
```

Arguments

data	data matrix or data frame
method	c("Pearson", "Spearman", "Kendall")
cor.thr	a threshold of correlation coefficient (default: $r \geq 0.6$)
neg.flag	flag where uses or not negative correlations
node.col	specifies color of nodes in a graph (default: red)
node.size	specifies size of nodes in a graph (default: 7)
edge.col	specifies color of edges in a graph (default: blue)
edge.width	specifies width of edges in a graph (default: 3)

Value

igraph object

Author(s)

Atsushi Fukushima

Examples

```
library(igraph)  
mat <- matrix(runif(100), nr=10)  
rownames(mat) <- as.character(1:10)  
generate_g(mat)
```

get.eigen.molecule *Get eigen molecule*

Description

Get eigen molecule

Usage

```
get.eigen.molecule(data, groups, whichgroups = NULL, methods = "svd", n = 10)
```

Arguments

data	a data matrix ([data.frame object] row: molecules, col: samples or replicates)
groups	a vector of group memberships as returned by cutree
whichgroups	a vector of group numbers to examine
methods	c("svd", "nipals", "rnipals", "bpca", "ppca"). See also pca() function in pcaMethods package
n	top n principal components

Value

the resulting vector.

Author(s)

Atsushi Fukushima

Examples

```
library(pcaMethods)
data(golub, package = "multtest")
hc.mol1 <- cluster.molecule(golub[1:100, 1:27], "pearson", "average")
g1 <- cutree(hc.mol1, h=0.6)
res1 <- get.eigen.molecule(golub[1:100,], g1)
```

```
get.eigen.molecule.graph
```

Getting graph from eigengene module list

Description

Getting graph from eigengene module list

Usage

```
get.eigen.molecule.graph(eigen.list, label = "Module")
```

Arguments

<code>eigen.list</code>	the resulting vector from <code>get.eigen.molecule</code>
<code>label</code>	a label of module extracted (default: "Module")

Value

igraph object

Author(s)

Atsushi Fukushima

Examples

```
library(pcaMethods)
library(igraph)
data(golub, package = "multtest")
hc.mol1 <- cluster.molecule(golub[, 1:27], "pearson", "average")
g1 <- cutree(hc.mol1, h=0.4)
res1 <- get.eigen.molecule(golub, g1)
g1.eigen <- get.eigen.molecule.graph(res1)
```

```
get.lfdr
```

Getting local false discovery rate (lfdr)

Description

Getting local false discovery rate (lfdr) using 'fdrtool' package

Usage

```
get.lfdr(r)
```

Arguments

`r` a vector of correlation coefficient under condition

Value

list of lfdr

Author(s)

Atsushi Fukushima

References

Strimmer, K. *Bioinformatics* (2008) 24, 1461-1462

Examples

```
library("fdrtool")
data(pvalues)
get.lfdr(pvalues)
```

`get.min.max`

Get minimum and maximum

Description

Get minimum and maximum

Usage

```
get.min.max(d)
```

Arguments

`d` data matrix or data frame

Value

list object of minimum value or maximum value in a data

Author(s)

Atsushi Fukushima

Examples

```
get.min.max(iris[,1:2])
```

golub.df

A compiled expression data from Golub et al. (1999)

Description

Golub data set from CoXpress paper by Michael Watson.

Details

This is a data.frame of AML/ALL leukaemia microarray study, originally from Golub et al Science 286:531 (1999). It comprises gene expression measurements from 38 tumor mRNA samples, including 27 cases of acute lymphoblastic leukemia (ALL) and 11 cases of acute myeloid leukemia (AML). The HU6800 Affymetrix array, which contains 6,800 probe sets, was used. The dataset was filtered to remove genes with negative values in any sample, resulting in a final set of 2,568 genes.

References

Michael Watson, BMC Bioinformatics 2006 7:509.

plotClusterMolecules *Plot cluster molecules*

Description

Plot cluster molecules

Usage

```
plotClusterMolecules(  
  data,  
  groups = NULL,  
  group.no = NULL,  
  title = NULL,  
  ylim = NULL,  
  order = NULL,  
  scale.center = FALSE,  
  scale.scale = FALSE,  
  frame = "white",  
  col = NULL,  
  bottom.mar = 5,  
  xlab = "Samples",  
  ylab = "Relative abundance"  
)
```

Arguments

<code>data</code>	data matrix or data frame
<code>groups</code>	a vector of group memberships as returned by <code>cutree</code>
<code>group.no</code>	the group number to be plotted
<code>title</code>	a title for the graph
<code>ylim</code>	a vector indicating the upper and lower limit for the y-axis
<code>order</code>	whether or not to order the columns of the data matrix
<code>scale.center</code>	unless NULL, each row is scaled using <code>scale</code>
<code>scale.scale</code>	unless NULL, each row is scaled using <code>scale</code> .
<code>frame</code>	the color of the frame that is drawn as the background of the plot
<code>col</code>	If NULL, all genes will be drawn in the default color (blue). If the text "random" is given, then a set of colors will be generated by
<code>bottom.mar</code>	The size of the bottom margin of the plots as sent in <code>par(mar=c(...))</code>
<code>xlab</code>	a label of x axis (default: "Samples")
<code>ylab</code>	a label of y axis (default: "Relative abundance")

Value

a graph

Author(s)

Atsushi Fukushima

References

this function was originally from Watson M (2005) BMC Bioinformatics 7:509

Examples

```
library(pcaMethods)
data(golub, package = "multtest")
hc.mol1 <- cluster.molecule(golub[, 1:27], "pearson", "average")
g1 <- cutree(hc.mol1, h=0.4)
plotClusterMolecules(golub[,1:27], g1, 3)
```

plotDiffCorrGroup *Plot DiffCorr group*

Description

Plot DiffCorr group

Usage

```
plotDiffCorrGroup(
  data,
  groups1 = NULL,
  groups2 = NULL,
  group1.no = NULL,
  group2.no = NULL,
  g1,
  g2,
  g1.order = NULL,
  g2.order = NULL,
  title1 = NULL,
  title2 = NULL,
  ...
)
```

Arguments

data	a data matrix or data frame
groups1	a vector of row group membership as produced by cutree under condition 1
groups2	a vector of row group membership as produced by cutree under condition 2
group1.no	the group number to be plotted (condition 1)
group2.no	the group number to be plotted (condition 2)
g1	a vector describing the columns of the data belonging to condition 1
g2	a vector describing the columns of the data belonging to condition 2
g1.order	whether or not to order the columns of the data matrix for condition 1. If "average", then the columns are ordered by the average expression value. If the name of a gene (row), then the columns are orderd according to the expression levels of that gene. If NULL, columns remain in their original order.
g2.order	See g1.order
title1	A title for the left hand graph
title2	A title for the right hand graph
...	other parameters to be passed to this function

Value

a graph

Author(s)

Atsushi Fukushima

Examples

```
library(pcaMethods)
data(golub, package = "multtest")
hc.mol1 <- cluster.molecule(golub[, 1:27], "pearson", "average")
hc.mol2 <- cluster.molecule(golub[, 28:38], "pearson", "average")
g1 <- cutree(hc.mol1, h=0.4)
g2 <- cutree(hc.mol2, h=0.4)
##
plotDiffCorrGroup(golub, g1, g2, 21, 24, 1:27, 28:38,
                  scale.center=TRUE, scale.scale=TRUE,
                  ylim=c(-5,5))
```

scalingMethods

scalingMethods

Description

The pre-treatment methods

Usage

```
scalingMethods(
  data,
  methods = c("auto", "range", "pareto", "vast", "level", "power")
)
```

Arguments

data a data matrix ([data.frame object] row: molecules, col: samples or replicates)
methods the chosen methods.

Value

the resulting data frame (or scaled data matrix)

Author(s)

Atsushi Fukushima

Examples

```
scalingMethods(iris[,1:4], "level")
```

uncent.cor2dist *Additional distance functions correlation distance (uncentered)*

Description

Additional distance functions correlation distance (uncentered)

Usage

```
uncent.cor2dist(data, i, absolute = FALSE)
```

Arguments

data	a data matrix ([data.frame object] row: metabolites, col: samples or replicates)
i	i-th row of data
absolute	TRUE means that absolute value of the correlation coefficient is used (Default: FALSE).

Details

These functions were originally from 'hybridHclust' package. We modified the functions slightly. See also the reference manual in detail.

Value

the resulting correlation matrix

Author(s)

Atsushi Fukushima

Examples

```
uncent.cor2dist(as.matrix(t(iris[,1:4])), 1) ## NOT RUN!
```

uncent.cordist *Calculating all pairwise distances using correlation distance*

Description

Calculating all pairwise distances using correlation distance

Usage

```
uncent.cordist(data, absolute = FALSE)
```

Arguments

data a data matrix ([data.frame object] row: metabolites, col: samples or replicates)
absolute TRUE means that absolute value of the correlation coefficient is used (Default: FALSE).

Details

These functions were originally from 'hybridHclust' package. We modified the functions slightly. See also the reference manual in detail.

Value

the resulting correlation matrix

Author(s)

Atsushi Fukushima

Examples

```
uncent.cordist(as.matrix(t(iris[,1:4]))) ## NOT RUN!
```

write.modules

Writing modules into a text file

Description

Writing modules into a text file

Usage

```
write.modules(cutree.res, mod.list, outfile = "module_list.txt")
```

Arguments

cutree.res the result of cutree function
mod.list the result of get.eigen.molecule
outfile file name of output

Value

a text file

Author(s)

Atsushi Fukushima

Examples

```
## Not run:  
data(golub, package = "multtest")  
hc.mol1 <- cluster.molecule(golub[, 1:27], "pearson", "average")  
g1 <- cutree(hc.mol1, h=0.4)  
res1 <- get.eigen.molecule(golub, g1)  
write.modules(g1, res1)  
  
## End(Not run)
```

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